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Deterministic Methods for Radiation Transport: Lessons Learned and Future Directions

Paul Nowak

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Deterministic Methods for Radiation Transport: Lessons Learned and Future Directions

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and Modern Software Practice**
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Paul Nowak
LLNL, AX -Division
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Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551 -0808

Solvers, solvers, solvers...



- **More robust and rapidly converging solution techniques will have the greatest impact**
- **The credibility of the “state -of-the-art” transport method has been established through extensive V&V**
- **Historically advances in algorithms have been far more important than advances in computer hardware**
- **Share our experiences with respect to discretization, iteration strategy and radiation -hydrodynamic coupling**

Withineach timestep, wesolveanonlinear problem



- Two equations are coupled linearly in the radiation intensity ψ , but nonlinearly in material temperature T
 - Boltzmann equation describes radiation transport: emission source is proportional to T^4
 - Energy balance for the material: temperature change is given by the net difference between absorption (proportional to ψ) and emission (proportional to T^4)
- It is possible to linearize the emission term (“linear semi-implicit”)
 - Overly constrains the timestep in real applications
 - Difficulty in getting the radiation and the matter to equilibrate
 - Accuracy and not a stability issue
 - Similar problems observed in IMC with its linearization

We use anested iteration to solve the nonlinear problem



Temperature Iteration

Emission Source
 $B(\nu, T) = b(\nu, T) * T^4$

Intensity Iteration

Newton Solve for T
 $T = f(T^4, \psi)$

T Converged?

Intensity Iteration

Sweep grid for all
Directions, groups
Given $B(\nu, T)$

GTASolve

ψ Converged?

GTASolve

BICGSTAB
"Action" =
1 Grey, S_2 sweep +
6-direction
"stretched" sweep
(no scattering)

Parallelsweepsareachallenge



- **Highly sensitive to partitioning**
 - METIS-like partitioning is death
 - Re-entrant and disjoint subdomains create inter-domain cycles
 - Lose the ability to match single process results in parallel
- **Block Iterative Methods**
 - Block Jacobi or Gauss-Seidel utilize all processors simultaneously
 - Convergence is slower compared to single-process
 - Observed penalty is typically 2X for small runs (that fit on a single process)
 - Penalty is unknown and much higher for “massively” parallel runs
 - Probably contribute to instability

Parallel Sweeps are a challenge con't



- **Scheduling**
 - **Honormore inter -domain dependencies**
 - **Need to idle processors**
 - **Smaller and more frequent messages**
 - **Greatly reduce iteration counts, but speedups are modest (~15%) due to the loss of parallelism**
 - **No efficient schedulers for Metis partitionings (Tri-Lab “Parallel S_N Project” at TAMU is working this issue)**
- **Where do we go from here?**
 - **Krylov Methods**

We have had success using Krylov methods in the grey acceleration step



- Used to solve the transport synthetic acceleration (TSA) equations
 - Grey and S_2 quadrature
 - Purely absorbing, 6 ordinate preconditioner
 - BCGSTAB or GMRES
 - Matrix free
 - Handles strongly heterogeneous problems
 - Reference: “Stretched and Filtered Preconditioning of SN Problems, Parts 1 & 2,” Hanshaw, Nowak, Larsen, *Trans Am. Nucl. Society*
- A similar approach could be used for DSA
 - May relax the consistency constraint

We are extending the use of Krylov methods to solving the multigroup, S_N equations directly



- Solve the nonlinear problem directly using Newton -Krylov
 - KINSOL package from CASC in collaboration with Keith Grant
- Memory Requirements
 - Storing multiple copies of the full angle -dependent intensity would be onerous
 - Use scalar intensity + boundary angular intensities as the solution vector
- Preconditioning
 - Initially, use a grey preconditioner
 - Can symmetric preconditioners work?
 - Do effective sweep-free preconditioners exist?

Report findings at NECDC 2004

Spatial discretization: “upstream” corner - balance* is effective on arbitrary grids



- **Unstructured Grids – Improvements needed**
 - **Positivity: negative fluxes may be amplified over time and during the nonlinear solve**
 - **Physically reasonable behavior on a skewed mesh, but not as critical when using ALE**
 - **Adaptive: detect and resolve boundary layers**
 - **Mixed-cell treatment**
- **Structured AMR Grids**
 - **One spatial unknown per cell – typically need factor of 10 to 100 more zones (Explicit Slope Method – Hanshaw, Larsen)**
 - **Coarser grid (compared to hydro) for radiation?**

* Subcell Balance Methods for Radiative Transfer on Arbitrary Grids, M.L. Adams, TTSP 1997

What about ray effects?

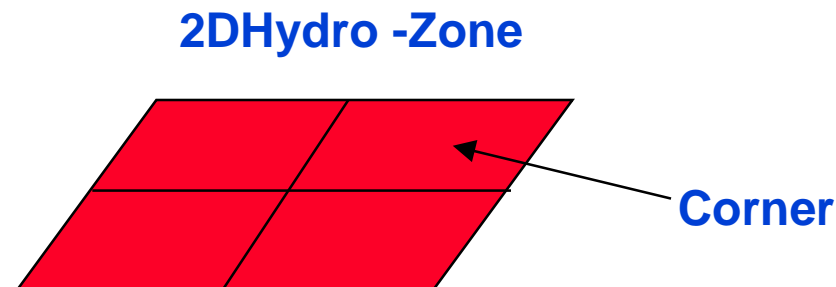


- Not an issue for most stockpile and AGEX applications
 - Sources are distributed
 - Typical figures of merit have shown to be weakly sensitive to angular discretization
 - Tailored quadrature sets work well for special cases (e.g. product quadrature sets with more forward -directed rays)
- An issue for ICF?

S_N +ALE Coupling: challenge is to remap large numbers of radiation variables effectively



- Transport and hydrodynamics use an unstructured grid
 - Each hydro -zone is composed of sub -zone volumes (“corners”) used in the transport discretization



- Remap occurs at the hydro -zone level
- Preserving the spatial distribution within a zone is important
 - Typically > 10,000 unknowns per zone ($\psi_{c,m,g}$)

Radiation and hydrodynamic coupling continue to be an “art”



- **Proper way to handle different centerings of hydro and radiation variables**
 - **Corner unknowns (e.g. temperatures) are scaled to match new zone-average values after hydro**
 - **Maintains intra-zone shape**
 - **Easier to maintain positivity**
- **Mixed-material zones**
 - **Depositing radiation energy in a mixed-material zone**
 - **Mixed-cell capacities**
 - **Can we make better use of interface information?**
- **Anticipating and treating excursions from “normal” physics regimes**
 - **Most frequent cause of “crashes”**

Great progress has been achieved, but more advances are needed



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